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INTERNAL REPORT

METHOD OF CALCULATING VARIANCES AND COVARIANCES FROM THE FUNDAMENTAL DEFINITION OF THESE QUANTITIES AND THE LAW FOR THE PROPAGATION OF ERRORS

BY

B. J. Dalton

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BRANCH Fundamental Research

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METHOD OF CALCULATING VARIANCES AND COVARIANCES FROM THE FUNDAMENTAL DEFINITION OF THESE QUANTITIES AND THE LAW FOR THE PROPAGATION OF ERRORS

by

B. J. Dalton[1/] and Robert E. Barieau[2/]

ABSTRACT

This report gives the mathematically exact equation for calculating all variances and covariances of the constants evaluated which is applicable to <u>any</u> function, regardless of the relationship between the observables and the constants, and was developed from the fundamental definition of these quantities and the law for the propagation of errors.

INTRODUCTION

As far as we are aware, all authors and all programs available for calculating variances and covariances are based on the assumption that the formulas that apply to linear problems are applicable to non-linear problems, <u>once</u> the linearized normal equations are

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formed. We reject this assumption, preferring to calculate variances and covariances from the fundamental definition of these quantities and the law for the propagation of errors (4, 6)[3/].

3/ Underlined numbers in parentheses refer to items in the list of references at the end of this report.

The present method in use for evaluating variances and covariances of the parameters is therefore only an approximation. How good this approximation is can only be decided by testing it against the mathematically exact equation to be given in this report. This exact equation is applicable to any function regardless of the relationship between the observables and the constants.

EVALUATION OF THE CONSTANTS

Let us consider a set of n experimental data points: $Y_{i(o)}$, x_{1_i}, x_{2_i}, x_{3_i}, ... (i=1,2, ... ,n), where $Y_{i(o)}$ is the $i^{\underline{th}}$ observed dependent variable and x_{j_i} (j=1,2, ... ,k) are the $i^{\underline{th}}$ observed independent variables. We define

$$F = F(Y_i; x_{j_i}; \beta_m) = 0 \qquad (1)$$

In our treatment of this problem, we assume that the x_{j_i}'s are accurately known and that random errors occur only in the observed Y_i's, and that they are normally distributed.

Now because of random errors in $Y_{i(o)}$, when $Y_{i(o)}$ is substituted in equation (1), F will not reduce exactly to zero. Let F_i be the

value of F when $Y_{i(o)}$ and x_{j_i} are substituted in equation (1); thus,

$$F_i = F(Y_{i(o)};\ x_{j_i};\ \beta_m) \tag{2}$$

Equation (1) can be solved for a <u>calculated</u> Y_i so that F reduces to zero; thus,

$$F = F(Y_{i(calc)};\ x_{j_i};\ \beta_m) = 0 \tag{3}$$

where x_j are the independent variables, corresponding to the observed x_j's evaluated at the $i^{\underline{th}}$ data point and β_m (m=1,2, ... ,k) are the k constants.

Now ΔY_i, the residual of $Y_{i(o)}$, is the difference between the observed and calculated values. This is not the true random error of $Y_{i(o)}$ because we do not know the true value of $Y_{i(o)}$. However, we can maximize the probability that the ΔY_i's are equal to the true random errors and this is just what the principle of least squares does. The principle of least squares says that we maximize the probability that the ΔY_i's represent the true random errors by minimizing the sum of the weighted squares of the residuals. Thus, we should minimize the quantity

$$R = \sum_{i=1}^{n} W_{Y_{i(o)}} (\Delta Y_i)^2 \tag{4}$$

where $W_{Y_{i(o)}}$ is the weight to be given $Y_{i(o)}$. If the $Y_{i(o)}$'s all have the same precision index, then they will have the same weight

and $W_{Y_{i(o)}} = 1$. If the $Y_{i(o)}$'s do not have the same precision index, then

$$W_{Y_{i(o)}} = \frac{L^2}{S^2_{Y_{i(o)}Y_{i(o)}}} \tag{5}$$

where L is a constant and $S^2_{Y_{i(o)}Y_{i(o)}}$ is the variance of $Y_{i(o)}$. In a particular problem, it may be necessary to assume $W_{Y_{i(o)}} = 1$ in the beginning; however, if this is done, then the residuals should be examined to see if there is any statistical evidence of the residuals squared being a function of the $Y_{i(o)}$'s. Any assumption as to the variance being a function of $Y_{i(o)}$ can be checked by examining the residuals. In any event, $W_{Y_{i(o)}}$ is not a function of the parameters to be evaluated.

To minimize R with regard to the various constants, we form the k partial derivative equations from which the k unknown constants can be obtained. Thus, we have a system of normal equations of the form

$$\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} = 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} = 0 \tag{6.1}$$

$$\left(\frac{\partial R}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} = 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} = 0 \tag{6.2}$$

$$\ldots \qquad \ldots \qquad \ldots$$

$$\left(\frac{\partial R}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots, \beta_{k-1}} = 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots, \beta_{k-1}} = 0 \qquad (6.k)$$

If the functional relationship between the observables and the constants is a linear one, then the solutions of the normal equations will be straightforward; however, if the functional relationship between these quantities is a non-linear one, then it will be necessary to solve the normal equations by an iterative procedure. Even though it may be necessary to solve the normal equations by a series of approximations, it is important to realize that the best values of the constants are determined such that the normal equations are satisfied exactly.

The method used by the Helium Research Center for handling non-linear regression problems is the Newton-Raphson method (7). In this method, the exact normal equations are formed and the problem is linearized by expanding the exact normal equations in a Taylor's series expansion, retaining the first two terms. For a more detailed discussion of the principles involved in non-linear regression problems, we refer the reader to our previous reports on this subject (1, 2).

The linearized normal equations are of the form

$$a_{11}\Delta\beta_1 + a_{12}\Delta\beta_2 + \ldots + a_{1k}\Delta\beta_k = \mu_1 \qquad (7.1)$$

$$a_{21}\Delta\beta_1 + a_{22}\Delta\beta_2 + \ldots + a_{2k}\Delta\beta_k = \mu_2 \qquad (7.2)$$

$$\ldots \qquad \ldots \qquad \ldots$$

$$a_{k1}\Delta\beta_1 + a_{k2}\Delta\beta_2 + \ldots + a_{kk}\Delta\beta_k = \mu_k \qquad (7.k)$$

where

$$a_{11} = \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)^{o^2}_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_1^2}\right)^{o}_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \qquad (8.11)$$

$$a_{21} = a_{12} = \left[\sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)^{o}_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)^{o}_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_1 \partial \beta_2}\right)^{o}_{x_{j_i}, Y_{i(o)}} \right] \qquad (8.12)$$

$$a_{k1} = a_{1k} = \left[\sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)^{o}_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)^{o}_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_1 \partial \beta_k}\right)^{o}_{x_{j_i}, Y_{i(o)}} \right] \qquad (8.1k)$$

$$a_{22} = \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)^{o^2}_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_2^2}\right)^{o}_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots} \qquad (8.22)$$

$$a_{k2} = a_{2k} = \left[\begin{array}{l} \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots} \\ + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_2 \partial \beta_k}\right)^o_{x_{j_i}, Y_{i(o)}} \end{array}\right] \quad (8.2k)$$

$$a_{kk} = \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)^{o^2}_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_k^2}\right)^o_{x_{j_i}, Y_{i(o)}} \quad (8.kk)$$

and

$$\mu_1 = -\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \quad (9.1)$$

$$\mu_2 = -\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} \quad (9.2)$$

$$\mu_k = -\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots, \beta_{k-1}} \quad (9.k)$$

and $\Delta\beta_1$, $\Delta\beta_2$, ..., $\Delta\beta_k$ are corrections to the undetermined parameters.

Equations (6.1), (6.2), ..., (6.k) result from expanding ΔY_i,

$$\left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}, \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots}, \ldots,$$

$\left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots, \beta_{k-1}}$ in a Taylor's series expansion about the approximate solution, $(\Delta Y_i)^o$, retaining only the first two terms.

The method to be used for obtaining the solutions of our linearized normal equations involves finding the inverse matrix, which we now proceed to do.

Let A represent the matrix of the coefficients of the linearized normal equations

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ & \cdot & \cdot & \cdot \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix}$$

or

$$A = [a_{jm}]_{(k,k)} = [a_{mj}]_{(k,k)} = A^T \qquad (10)$$

where

$$a_{jm} = \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_j}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_{m \neq j}} \left(\frac{\partial \Delta Y_i}{\partial \beta_m}\right)^o_{x_{j_i}, Y_{i(o)}, \beta_{j \neq m}} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i^o \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_j \partial \beta_m}\right)^o_{x_{j_i}, Y_{i(o)}} \qquad (11)$$

Here, j ranges from 1 to k and denotes the row, while m ranges from 1 to k and denotes the column of the element a_{jm}, and A^T of order

(k,k), obtained by interchanging rows and columns in matrix A of order (k,k), is referred to as the transpose of A.

Now let us write the linearized normal equations as the single matrix equation

$$[a_{jm}]_{(k,k)}[\Delta\beta_m]_{(k,1)} = [\mu_j]_{(k,1)} \tag{12}$$

where $[\Delta\beta_m]_{(k,1)}$ is a column matrix of k rows, and $[\mu_j]_{(k,1)}$ is a column matrix of k rows.

Let b_{jm} represent the elements of the inverse matrix, designated as A^{-1},

$$A^{-1} = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1k} \\ b_{21} & b_{22} & \cdots & b_{2k} \\ \cdot & \cdot & & \cdot \\ b_{k1} & b_{k2} & \cdots & b_{kk} \end{bmatrix}$$

or

$$A^{-1} = [b_{jm}]_{(k,k)} = [b_{mj}]_{(k,k)} = (A^{-1})^T \tag{13}$$

Now A^{-1} is just that matrix which when multiplied by A gives the identity matrix, I

$$A^{-1}A = I$$

$$= \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ & \cdot & \cdot & \cdot \\ 0 & 0 & \cdots & 1 \end{bmatrix}_{(k,k)} \tag{14}$$

and we see from equation (14) that the identity matrix ... "is uniquely defined by the property that it behaves like the scalar 1 in matrix multiplication" (5). Therefore, multiplying both sides of equation (12) by A^{-1}, we get

$$[\Delta\beta_m]_{(k,1)} = [b_{jm}]_{(k,k)}[\mu_j]_{(k,1)}$$

$$= [b_{mj}]_{(k,k)}[\mu_j]_{(k,1)} \tag{15}$$

from which we can evaluate the $\Delta\beta_m$'s, where the $\Delta\beta_m$'s (m=1, 2, ..., k) are defined as

$$\Delta\beta_1 = \beta_1 - \beta_1^o \tag{16.1}$$

$$\Delta\beta_2 = \beta_2 - \beta_2^o \tag{16.2}$$

$$\cdots \quad \cdots$$

$$\Delta\beta_k = \beta_k - \beta_k^o \tag{16.k}$$

and $\beta_1, \beta_2, \ldots, \beta_k$ are the undetermined constants while $\beta_1^o, \beta_2^o, \ldots, \beta_k^o$ are approximate values for these quantities.

If the assumed values for the undetermined constants are not too good, then it will be necessary to repeat the calculations using the new $\beta_1, \beta_2, \ldots, \beta_k$ as the start of a new iteration. We continue this iterative technique, <u>provided</u> the problem is continuing to converge, until $\mu_1 = \mu_2 = \ldots = \mu_k = 0$, to within some predetermined small quantity, the final $\beta_1, \beta_2, \ldots, \beta_k$ being the least squares solution for these quantities. For a more detailed discussion of methods to use that will lead to convergence of the

iteration when the problem starts diverging, we refer the reader to our previous report (3) on this subject.

CALCULATION OF VARIANCES AND COVARIANCES

Once we have determined the best values of β_1, β_2, ..., β_k, we proceed to calculate all variances and covariances of these constants. We do this from the fundamental definition of these quantities and the law for the propagation of errors (4, 6).

This law says that if we have a function or quantity, say Q, that is a function of the independently-observed quantities y_1, y_2, ..., y_n, then the variance of Q is given as

$$S^2_{QQ} = \sum_{i=1}^{n} \left(\frac{\partial Q}{\partial y_{i(o)}}\right)^2 S^2_{y_{i(o)}y_{i(o)}} \tag{17}$$

where $S^2_{y_{i(o)}y_{i(o)}}$ is the variance of $y_{i(o)}$, and S^2_{QQ} is the variance of Q. Extracting the square root of the variance, we obtain a value on the same scale as the function Q. This value is referred to as the standard error or standard deviation of Q.

The values of our constants which we have evaluated are functions of all of the observed Y_i's and x_{j_i}'s. Since we assumed the errors of the x_{j_i}'s to be zero, then the expression for calculating the <u>variances</u> of the constants is of the form

$$S^2_{\beta_m\beta_m} (m=1, 2, \ldots, k) = \sum_{i=1}^{n} \left(\frac{\partial \beta_m}{\partial Y_{i(o)}}\right)^2 S^2_{Y_{i(o)}Y_{i(o)}} \tag{18}$$

[illegible]

[illegible]

$$[illegible]$$

[illegible]

[illegible]

$$[illegible]$$

The expression for calculating the covariances of the constants is of the form

$$S^2_{\beta_m\beta_j}(j=1,\ 2,\ \ldots\ k;\ j\neq m) = \sum_{i=1}^{n}\left(\frac{\partial\beta_m}{\partial Y_{i(o)}}\right)\left(\frac{\partial\beta_j}{\partial Y_{i(o)}}\right)S^2_{Y_{i(o)}Y_{i(o)}} \qquad (19)$$

Now in order to evaluate equation (18), we must evaluate $\left(\frac{\partial\beta_m}{\partial Y_{i(o)}}\right)$(m=1, 2, ... k), multiply by $S_{Y_{i(o)}Y_{i(o)}}$, square the product of these two quantities and then sum the resulting product over all of the observed Y_i's. Similarly, in order to evaluate equation (19), we need to evaluate $\left(\frac{\partial\beta_m}{\partial Y_{i(o)}}\right)$(m=1, 2, ... k) and $\left(\frac{\partial\beta_j}{\partial Y_{i(o)}}\right)$(j=1, ..., k; j≠m), multiply the product of these two quantities by $S^2_{Y_{i(o)}Y_{i(o)}}$, then sum the resulting product over all of the $Y_{i(o)}$'s. We now proceed to evaluate these quantities.

We have a total of n pairs of the observed quantities Y_i, x_{j_i}. The constants are determined from the solutions of equations (6.1), (6.2), ..., (6.k). Now suppose we change one of the observed Y_i's, say $Y_{2(o)}$, to $[Y_{2(o)} + \Delta Y_{2(o)}]$. Then on solving equations (6.1), (6.2), ..., (6.k), we will get new values of β_1, β_2, ..., β_k. Then we can calculate

$$\left(\frac{\partial\beta_m}{\partial Y_{2(o)}}\right) = \frac{\Delta\beta_m}{\Delta Y_{2(o)}}\ (m=1,\ 2,\ \ldots\ k) \qquad (20)$$

This means that when we change $Y_{2(o)}$ by the small amount $\Delta Y_{2(o)}$, then equations (6.1), (6.2), ..., (6.k) must still hold exactly.

Mathematically, this means that

$$\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} = 0 \quad (m=1,\ 2,\ \ldots,k) \tag{21}$$

Now the $\left(\frac{\partial R}{\partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}}$'s are functions of all of the constants and, through the constants evaluated, are functions of all of the $Y_{i(o)}$'s. Then, under these conditions, we have

$$\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}} = \left[\begin{array}{l} \displaystyle\sum_{m=1}^{k}\left(\frac{\partial \beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\left(\frac{\partial^2 R}{\partial \beta_1 \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \\ \displaystyle + \left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} \end{array}\right] \tag{22.1}$$

$$\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots}\right]_{x_{j_i}, Y_{r\neq i}} = \left[\begin{array}{l} \displaystyle\sum_{m=1}^{k}\left(\frac{\partial \beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\left(\frac{\partial^2 R}{\partial \beta_2 \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \\ \displaystyle + \left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} \end{array}\right] \tag{22.2}$$

. . .

$$\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}} = \left[\begin{array}{l} \sum_{m=1}^{k}\left(\frac{\partial \beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\left(\frac{\partial^2 R}{\partial \beta_k \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \\ + \left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} \end{array}\right] \tag{22.k}$$

Now we can solve equations (22.1), (22.2), ..., (22.k) simultaneously and evaluate the derivatives $\left(\frac{\partial \beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}$, $\left(\frac{\partial \beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}$, ..., $\left(\frac{\partial \beta_k}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}$. Then once we have expressions for each of these quantities, we can multiply each derivative, say $\left(\frac{\partial \beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}$, by $S_{Y_{i(o)}Y_{i(o)}}$, square the product, then sum this product over all of the observed Y_i's. This will give us an expression from which we can calculate the variance of β_1. In a like manner, we can calculate the variance of β_2, of β_3, ..., and of β_k.

In order to evaluate the variances of our constants, we see from equations (22.1), (22.2), ..., (22.k) that we need expressions for $\left(\frac{\partial^2 R}{\partial \beta_1 \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}}$, $\left(\frac{\partial^2 R}{\partial \beta_2 \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}}$, ..., $\left(\frac{\partial^2 R}{\partial \beta_k \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}}$ and for $\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots}$, $\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots}$, ..., $\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots, \beta_{k-1}}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots}$. We now proceed

to evaluate these quantities.

We start with equations (6.1), (6.2), ..., (6.k):

$$\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} = 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \quad (6.1)$$

$$\left(\frac{\partial R}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} = 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} \quad (6.2)$$

$$\cdots$$

$$\left(\frac{\partial R}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_2, \ldots} = 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_2, \ldots} \quad (6.k)$$

Let us differentiate equation (6.1) with regard to each constant; thus,

$$\left(\frac{\partial^2 R}{\partial \beta_1 \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} = \left[\begin{array}{l} 2\sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \left(\frac{\partial \Delta Y_i}{\partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \\ + 2\sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_1 \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \end{array}\right] \quad (m=1,2,\ldots,k) \quad (23)$$

And differentiating equation (6.1) with regard to a single $Y_{i(o)}$, holding all constants and all x_{j_i}'s fixed, we get:

$$\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} = \tag{24}$$

$$\left[\begin{array}{l} 2W_{Y_{i(o)}}\left(\frac{\partial \Delta Y_i}{\partial Y_{i(o)}}\right)_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots}\left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \\ +2W_{Y_{i(o)}}\Delta Y_i\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} \end{array}\right]$$

Now ΔY_i, the residual of $Y_{i(o)}$, is just the difference between $Y_{i(o)}$ and $Y_{i(calc)}$. Therefore,

$$\left(\frac{\partial \Delta Y_i}{\partial Y_{i(o)}}\right)_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} = 1 \tag{25}$$

and

$$\left[\frac{\partial}{\partial \beta_1}\left(\frac{\partial \Delta Y_i}{\partial Y_{i(o)}}\right)_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots}\right]_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} = \left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} = 0 \tag{26}$$

Substituting equations (25) and (26) into equation (24), we get

$$\left[\frac{\partial}{\partial Y_{i(o)}}\left(\frac{\partial R}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots}\right]_{x_{j_i}, Y_{r\neq i}, \beta_1, \ldots} = 2W_{Y_{i(o)}}\left(\frac{\partial \Delta Y_i}{\partial \beta_1}\right)_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \tag{27}$$

Therefore, we have from equations (23), (27), (21), and (22.1):

$$a_{11}\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} + a_{12}\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} + \ldots + a_{1k}\left(\frac{\partial\beta_k}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} = M_1 \qquad (28.1)$$

where

$$a_{11} = \sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_1}\right)^2_{x_{j_i},Y_{i(o)},\beta_2,\ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}}\,\Delta Y_i\left(\frac{\partial^2\Delta Y_i}{\partial\beta_1^2}\right)_{x_{j_i},Y_{i(o)},\beta_2,\ldots} \qquad (29.11)$$

$$a_{12} = \sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_1}\right)_{x_{j_i},Y_{i(o)},\beta_2,\ldots}\left(\frac{\partial\Delta Y_i}{\partial\beta_2}\right)_{x_{j_i},Y_{i(o)},\beta_1,\beta_3,\ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}}\,\Delta Y_i\left(\frac{\partial^2\Delta Y_i}{\partial\beta_1\partial\beta_2}\right)_{x_{j_i},Y_{i(o)}} \qquad (29.12)$$

$$a_{1k} = \sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_1}\right)_{x_{j_i},Y_{i(o)},\beta_2,\ldots}\left(\frac{\partial\Delta Y_i}{\partial\beta_k}\right)_{x_{j_i},Y_{i(o)},\beta_1,\ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}}\,\Delta Y_i\left(\frac{\partial^2\Delta Y_i}{\partial\beta_1\partial\beta_k}\right)_{x_{j_i},Y_{i(o)}} \qquad (29.1k)$$

and

$$M_1 = -W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_1}\right)_{x_{j_i},Y_{i(o)},\beta_2,\ldots} \qquad (30.1)$$

Now differentiating equations (6.2), ..., (6.k) with regard to each constant and then with regard to a single $Y_{i(o)}$, we get expressions similar to equations (23) and (27). Then upon substituting these expressions into equations (22.2), ..., (22.k), recalling the relationship of equation (21), we get expressions similar to

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equation (28.1) of the form

$$a_{21}\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} + a_{22}\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} + \ldots + a_{2k}\left(\frac{\partial\beta_k}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} = M_2 \qquad (28.2)$$

$$\ldots \qquad\qquad \ldots$$

$$a_{k1}\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} + a_{k2}\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} + \ldots + a_{kk}\left(\frac{\partial\beta_k}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} = M_k \qquad (28.k)$$

where

$$a_{21} = a_{12} \qquad (29.12)$$

$$\ldots \qquad \ldots$$

$$a_{k1} = a_{1k} \qquad (29.1k)$$

$$a_{22} = \sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_2}\right)^2_{x_{j_i},Y_{i(o)},\beta_1,\beta_3,\ldots} + \sum_{i=1}^{n} W_{Y_{i(o)}}\Delta Y_i\left(\frac{\partial^2\Delta Y_i}{\partial\beta_2^2}\right)_{x_{j_i},Y_{i(o)},\beta_1,\beta_3,\ldots} \qquad (29.22)$$

$$a_{k2} = a_{2k} = \left[\begin{array}{l} \sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_2}\right)_{x_{j_i},Y_{i(o)},\beta_1,\beta_3,\ldots}\left(\frac{\partial\Delta Y_i}{\partial\beta_k}\right)_{x_{j_i},Y_{i(o)},\beta_1,\ldots} \\ + \sum_{i=1}^{n} W_{Y_{i(o)}}\Delta Y_i\left(\frac{\partial^2\Delta Y_i}{\partial\beta_2\partial\beta_k}\right)_{x_{j_i},Y_{i(o)}} \end{array}\right] \qquad (29.2k)$$

$$a_{kk} = \sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_k}\right)^2_{x_{j_i},Y_{i(o)},\beta_1,\ldots,\beta_{k-1}} + \sum_{i=1}^{n} W_{Y_{i(o)}}\Delta Y_i\left(\frac{\partial^2\Delta Y_i}{\partial\beta_k^2}\right)_{x_{j_i},Y_{i(o)}} \qquad (29.kk)$$

and

$$M_2 = -W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_2}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \beta_3, \ldots} \tag{30.2}$$

$$\ldots \qquad \ldots \qquad \ldots$$

$$M_k = -W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_k}\right)_{x_{j_i}, Y_{i(o)}, \beta_1, \ldots, \beta_{k-1}} \tag{30.k}$$

Equations (28.1), (28.2), ..., (28.k) can be written as the single matrix equation

$$A \left[\left(\frac{\partial \beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\right]_{(k,1)} = [M_j]_{(k,1)} \tag{31}$$

where

$$A = [a_{jm}]_{(k,k)} = [a_{mj}]_{(k,k)} = A^T \tag{32}$$

and

$$a_{jm} = \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_j}\right)_{x_{j_i}, Y_{i(o)}, \beta_{m\neq j}} \left(\frac{\partial \Delta Y_i}{\partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}, \beta_{j\neq m}} + \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_j \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \tag{33}$$

Here, j ranges from 1 to k and denotes the row, while m ranges from 1 to k and denotes the column of the element a_{jm}; $\left[\left(\frac{\partial \beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\right]_{(k,1)}$ is a column matrix of k rows; and $[M_j]_{(k,1)}$ is a column matrix of k rows.

We see that the a_{jm} element defined by equation (33) is of the same form as that defined by equation (11). The difference

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between these two definitions is that equation (33) applies when the least squares solution is obtained while equation (11) applies to a trial solution. For the final iteration, a_{jm} as defined by equation (33) can be considered as the value of the a_{jm} element of the coefficient matrix.

Multiplying equation (31) by the inverse matrix, A^{-1}, we get

$$\left[\left(\frac{\partial\beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\right]_{(k,1)} = A^{-1}[M_j]_{(k,1)} \tag{34}$$

where

$$A^{-1} = [b_{jm}]_{(k,k)} = [b_{mj}]_{(k,k)} = (A^{-1})^T \tag{35}$$

j ranging from 1 to k and identifies the row, while m ranges from 1 to k and denotes the column of the b_{jm} element. The b_{jm} element defined by equation (35) is of the same form as that defined by equation (13). The difference between these two definitions is that equation (35) applies when the least squares solution is obtained, whereas equation (13) applies to a trial solution. For the final iteration, b_{jm} of equation (35) can be considered as the value of the b_{jm} element of the inverse matrix.

Therefore, from equations (34) and (35), we have

$$\left[\left(\frac{\partial\beta_m}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\right]_{(k,1)} = [b_{mj}]_{(k,k)}[M_j]_{(k,1)} \tag{36}$$

and the derivative $\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}$ is of the form:

$$\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} = b_{11}M_1 + b_{21}M_2 + \ldots + b_{k1}M_k$$

$$= b_{11}M_1 + b_{12}M_2 + \ldots + b_{1k}M_k \tag{37}$$

Now multiplying equation (37) by $S_{Y_{i(o)}Y_{i(o)}}$ and then squaring this product, we have

$$\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)^2_{Y_{r\neq i}} S^2_{Y_{i(o)}Y_{i(o)}} = \begin{bmatrix} b_{11}^2M_1^2 + b_{12}^2M_2^2 + \ldots + b_{1k}^2M_k^2 \\ + b_{11}b_{12}M_1M_2 + b_{12}b_{11}M_1M_2 \\ + \ldots + b_{11}b_{1k}M_1M_k + b_{1k}b_{11}M_1M_k \\ + b_{12}b_{1k}M_2M_k + b_{1k}b_{12}M_2M_k \\ + \ldots \end{bmatrix} S^2_{Y_{i(o)}Y_{i(o)}} \tag{38}$$

But from equation (5)

$$S^2_{Y_{i(o)}Y_{i(o)}} = \frac{L^2}{W_{Y_{i(o)}}} \tag{39}$$

and multiplying equation (39) by M_1^2, where M_1 is defined by equation (30.1), we get

$$M_1^2\, S^2_{Y_{i(o)}Y_{i(o)}} = L^2\, W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_1}\right)^2_{x_{j_i}, Y_{i(o)}, \beta_2, \ldots} \tag{40}$$

and, in general,

$$M_m M_j S^2_{Y_{i(o)}Y_{i(o)}}\binom{m=1,2,\ldots,k}{j=1,2,\ldots,k} = L^2 W_{Y_{i(o)}}\left(\frac{\partial \Delta Y_i}{\partial \beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial \Delta Y_i}{\partial \beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}} \qquad (41)$$

Substituting equation (41) into equation (38) and then summing over all of the $Y_{i(o)}$'s, we get

$$\sum_{i=1}\left(\frac{\partial \beta_1}{\partial Y_{i(o)}}\right)^2 S^2_{Y_{i(o)}Y_{i(o)}} = S^2_{\beta_1\beta_1}$$

$$= L^2 \sum_{m=1}^{k}\sum_{j=1}^{k}\left[b_{1m}b_{1j}\sum_{i=1}^{n} W_{Y_{i(o)}}\left(\frac{\partial \Delta Y_i}{\partial \beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial \Delta Y_i}{\partial \beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}}\right] \qquad (42)$$

which is the mathematically exact equation for calculating the variance of β_1.

Now the derivative $\left(\frac{\partial \beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}$ is of the form

$$\left(\frac{\partial \beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} = b_{21}M_1 + b_{22}M_2 + \ldots + b_{2k}M_k \qquad (43)$$

Multiplying equation (43) by $S_{Y_{i(o)}Y_{i(o)}}$ and then squaring this product, we get

$$\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)^2_{Y_{r\neq i}} S^2_{Y_{i(o)}Y_{i(o)}} = \begin{bmatrix} b^2_{21}M^2_1 + b^2_{22}M^2_2 + \ldots + b^2_{2k}M^2_k \\ + b_{21}b_{22}M_1M_2 + b_{22}b_{21}M_2M_1 + \ldots \\ + b_{21}b_{2k}M_1M_k + b_{22}b_{2k}M_2M_k \\ + b_{2k}b_{22}M_2M_k + \ldots \end{bmatrix} S^2_{Y_{i(o)}Y_{i(o)}} \tag{44}$$

Substituting equation (41) into equation (44) and summing over all of the observed Y_i's, we get

$$\sum_{i=1}^{n}\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)^2 S^2_{Y_{i(o)}Y_{i(o)}} = S^2_{\beta_2\beta_2} \tag{45}$$

$$= L^2\sum_{m=1}^{k}\sum_{j=1}^{k}\left[b_{2m}b_{2j}\sum_{i=1}^{n}W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial\Delta Y_i}{\partial\beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}}\right]$$

which is the exact equation from which we can calculate the variance of β_2. Similarly, the variance of β_k is of the same form as β_1 and β_2:

$$S^2_{\beta_k\beta_k} = L^2\sum_{m=1}^{k}\sum_{j=1}^{k}\left[b_{km}b_{kj}\sum_{i=1}^{n}W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial\Delta Y_i}{\partial\beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}}\right] \tag{46}$$

Now we proceed to calculate the covariances of our constants. Suppose we multiply the product of equations (37) and (43) by $S^2_{Y_{i(o)}Y_{i(o)}}$. This gives us

$$\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}}\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)_{Y_{r\neq i}} S^2_{Y_{i(o)}Y_{i(o)}} = \left[\begin{array}{l} b_{11}b_{21}M_1^2 + b_{11}b_{22}M_1M_2 + \ldots + b_{11}b_{2k}M_1M_k \\ + b_{12}b_{21}M_2M_1 + b_{12}b_{22}M_2^2 + \ldots + b_{12}b_{2k}M_2M_k \\ + \ldots \\ + b_{1k}b_{21}M_kM_1 + b_{1k}b_{22}M_kM_2 + \ldots + b_{1k}b_{2k}M_k^2 \end{array}\right] S^2_{Y_{i(o)}Y_{i(o)}} \tag{47}$$

and substituting equation (41) into equation (47) and then summing over all of the $Y_{i(o)}$'s, we get

$$\sum_{i=1}\left(\frac{\partial\beta_1}{\partial Y_{i(o)}}\right)\left(\frac{\partial\beta_2}{\partial Y_{i(o)}}\right)S^2_{Y_{i(o)}Y_{i(o)}} = S^2_{\beta_1\beta_2}$$

$$= L^2\sum_{m=1}^{k}\sum_{j=1}^{k}\left[b_{1m}b_{2j}\sum_{i=1}^{n}W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial\Delta Y_i}{\partial\beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}}\right] \tag{48}$$

from which we can calculate the covariance of $\beta_1\beta_2$. Similarly, the covariance of $\beta_1\beta_q$ is of the form

$$S^2_{\beta_1\beta_q} = L^2\sum_{m=1}^{k}\sum_{j=1}^{k}\left[b_{1m}b_{qj}\sum_{i=1}^{n}W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial\Delta Y_i}{\partial\beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}}\right] \tag{49}$$

where b_{qj} is the element of the inverse matrix of order (k,k). Similarly, the covariance of $\beta_2\beta_q$ is of the form

$$S^2_{\beta_2\beta_q} = L^2\sum_{m=1}^{k}\sum_{j=1}^{k}\left[b_{2m}b_{qj}\sum_{i=1}^{n}W_{Y_{i(o)}}\left(\frac{\partial\Delta Y_i}{\partial\beta_m}\right)_{x_{j_i},Y_{i(o)},\beta_{j\neq m}}\left(\frac{\partial\Delta Y_i}{\partial\beta_j}\right)_{x_{j_i},Y_{i(o)},\beta_{m\neq j}}\right] \tag{50}$$

Therefore, we see from equations (42), (45), (46), (48), (49), and (50) that we can write the single equation

$$S^2_{\beta_p\beta_q} = L^2 \sum_{m=1}^{k} \sum_{j=1}^{k} \left[b_{pm} b_{qj} \sum_{i=1}^{n} W_{Y_{i(o)}} \left(\frac{\partial \Delta Y_i}{\partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}, \beta_{j\neq m}} \left(\frac{\partial \Delta Y_i}{\partial \beta_j}\right)_{x_{j_i}, Y_{i(o)}, \beta_{m\neq j}} \right] \tag{51}$$

where b_{pm} is the element of the inverse matrix of order (k,k). Equation (51) is the generalized exact equation from which we can calculate <u>all</u> variances and <u>all</u> covariances of the constants evaluated because if $p = q = 1$, then equation (51) is nothing but the expression for calculating the variance of β_1 and is just equation (42). Now if $p=1$ and $q=2$, then equation (51) is nothing but equation (48) and is the expression for calculating the covariance of $\beta_1\beta_2$.

Suppose we simplify equation (51) by substituting equation (33) into equation (51):

$$S^2_{\beta_p\beta_q} = L^2 \sum_{m=1}^{k} \sum_{j=1}^{k} b_{pm} b_{qj} a_{jm} - L^2 \sum_{m=1}^{k} \sum_{j=1}^{k} \left[b_{pm} b_{qj} \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_j \partial \beta_m}\right)_{x_{j_i}, Y_{i(o)}} \right] \tag{52}$$

From equation (32), we have

$$A = [a_{jm}]_{(k,k)} = [a_{mj}]_{(k,k)} = A^T \tag{32}$$

Let the inverse of A, designated as A^{-1}, be

$$A^{-1} = [b_{qj}]_{(k,k)} = [b_{jq}]_{(k,k)} = (A^{-1})^T \tag{53}$$

Then

$$A^{-1}A = I$$

$$= [c_{mq}]_{(k,k)} \tag{54}$$

where

$$c_{mq} = \sum_{j=1}^{k} a_{mj} b_{jq} \tag{55}$$

and it follows that $c_{mq}(m=q) = 1$ and $c_{mq}(m \neq q) = 0$. Therefore, we see that the first term which appears on the right-hand side of equation (52) is

$$\sum_{m=1}^{k} b_{pm} \left(\sum_{j=1}^{k} a_{mj} b_{jq} \right) = b_{pq} \tag{56}$$

Therefore, substituting equation (56) into equation (52), we get

$$S^2_{\beta_p \beta_q} = L^2 b_{pq} - L^2 \sum_{m=1}^{k} \sum_{j=1}^{k} \left[b_{pm} b_{qj} \sum_{i=1}^{n} W_{Y_{i(o)}} \Delta Y_i \left(\frac{\partial^2 \Delta Y_i}{\partial \beta_j \partial \beta_m} \right)_{x_{j_i}, Y_{i(o)}} \right] \tag{57}$$

which is the exact mathematical equation from which we can calculate <u>all</u> variances and covariances of the constants evaluated. Notice that since the coefficient matrix is symmetrical, then it is only necessary to evaluate half of the elements of the coefficient matrix <u>and</u> of the inverse matrix. In other words, we need only evaluate those elements which lie on or above the principal diagonal of A and of A^{-1} [The principal diagonal is composed of those elements which have the <u>same</u> row and column index].

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